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12-14 June 2007, at US Naval Academy, Annapolis, MD

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____

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Efficient Modeling & Simulation of Biological Warfare Using Innovative Design of Experiments Methods

Presented at

75th MORS Symposium

12, 13 & 14 June 2007

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Why Use Design of Experiments (DOE) Methods with Simulation Experiments?

Quicker answers, lower costs, solve bigger problems

- Obtain a fast and cheap surrogate “meta-model” of the simulation
  - can more rapidly answer “what if?” questions
  - do sensitivity analysis
- By running efficient subsets of all possible combinations, one can - for the same resources and constraints – solve bigger problems
- Be as cost effective as possible and run no more trials than are needed to get a useful answer

Summary

- Demonstrated how Design of Experiments (DOE) can be used to sequentially run groups of simulation trials to obtain better and better meta-models of the simulation model
- When control variables are all continuous and response variable is NON-stochastic, then "Smoothing" designs can be used to efficiently produce a meta-model of a simulation that is made up of a complex series of physical models

Two Types of Designs for Two Types of Meta-Modeling of Simulations

- **"Traditional" designs for polynomial modeling with categorical and continuous variables**
  - Designs can be sequentially constructed to support increasingly complex models
  - Featured example reanalyzes a simulation case matrix in which all 648 combinations of variable settings were originally run
- **"Smoothing" designs for use with continuous variables AND non-stochastic responses**
  - Though little used, these designs are a more efficient alternative to traditional designs and exploit "Kriging" regression analysis

Traditional Designs for Polynomial Modeling

- **If a "textbook" fractional-factorial, orthogonal array or response-surface design is available, then use it.**
- **Textbooks and web site catalogs do not always contain designs for categorical variables with:**
  - all combinations of mixed numbers of levels (e.g. 3, 4, 5, and 21)
  - large numbers of levels for variables (e.g. 5+)
- **Algebraic (**Orthogonal Array**) and algorithmic (**D-optimal**) computer generated designs can often be used**
  - Orthogonal Arrays are good at yielding analysis with "clean" (unconfounded) estimates of the "main effects"
  - D-optimal designs are good for adding on the fewest additional trials to support higher order "interaction" terms in the model

Case Matrix (TBM Bulk) & Example Dosage Plot as Used in Study of the Observed Response "Probability of Casualty" (PCAS)

Variable	# Levels	Levels
Agent Codes[1]	6	A, N, T, H, R, Y (categorical)
Season	3	Winter, Summer, Spring/Fall (categorical)
Time of Attack	3	0500, 1200, 2200 Local Time (continuous)
No. of TBMs & Spread Radius[2]	2	1 TBM & 1 m, 2 TBMs & 1000 m (categorical)
Mass[3,4] (relative)	3	1.00, 1.57, 2.00 (continuous)
Height of Burst[5]	2	0, 10 m (continuous)
Total Cases	648	

1. Dropped "Q" - it had smallest effect & 6 levels allowed for use of a smaller Orthogonal Array
2. Spread Radius paired with No. of TBMs
3. Mass (with 3 levels) replaced Source Strength (with 2 levels)
4. Mass is nested in Agent
5. Data was available for Height of 10 m

See Presentation by Dan Cinotti in WG-2, NBC Defense, 1100 on Thursday

Statistical Details

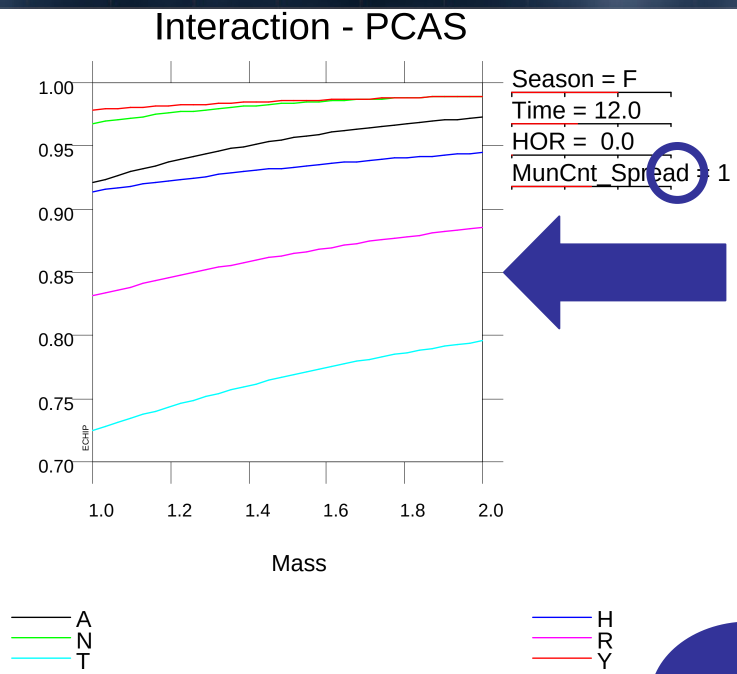
- **Because a different set of mass values were used for each agent, the variable Mass is "nested" within the variable Agent**
- **The response Probability of Casualty (PCAS), which is bounded within the range (0, 1), was transformed using $2*\text{Arcsin}((\text{PCAS})^{1/2})$ which maps the range (0, 1) to the range (-∞, +∞)**
  - This made the error fit the usual regression assumption of being normally distributed
  - This also prevented our regression from predicting values and limits that were above 1.0 and physically impossible

Four Stage Design Sequence

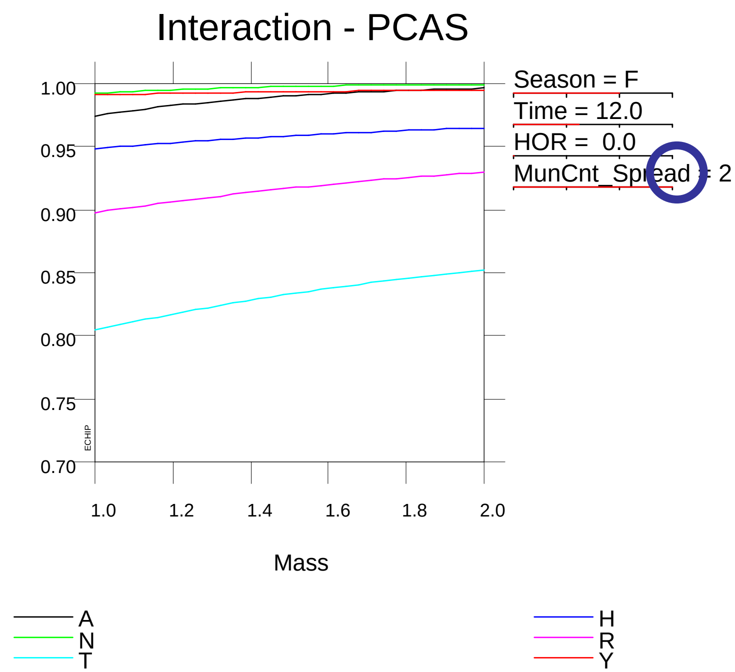
Stage 1	Stage 2	Stage 3	Stage 4
36 Total Simulations	**108** Total Simulations	**324** Total Simulations	ALL **648** Simulations
Design 1, 36 trials	Design 1, 36 trials	Design 1, 36 trials	Design 1, 36 trials
	Design 2, 72 trials	Design 2, 72 trials	Design 2, 72 trials
		Design 3, 216 trials	Design 3, 216 trials
Main effects only for ALL variables	Stage 1 effects plus all 2-way interactions	Stage 2 effects plus all 3-way interactions	Stage 3 effects plus ALL remaining 4-way, 5-way and 6-way interactions
5.6% of 648	16.7% of 648	50% of 648	Design 4, 324 trials NOTE: Length of this green box should be longer than shown

324 trials in Design 4 used as checkpoints for Designs 1, 2 & 3

Tabled (Categorical) vs. Plot (Continuous) Predictions of PCAS for 2nd Order Model



	1	1.5714	2
MunCnt_S =	1		
A	0.917	0.959	0.974
H	0.916	0.935	0.944
N	0.966	0.986	0.992
R	0.833	0.868	0.884
T	0.730	0.772	0.793
Y	0.980	0.986	0.989



	1	1.5714	2
MunCnt_S =	2		
A	0.977	0.991	0.995
H	0.947	0.960	0.966
N	0.993	0.998	0.999
R	0.895	0.920	0.931
T	0.802	0.837	0.854
Y	0.990	0.993	0.995

Predictions (w/95% Pred. Limits) of PCAS vs. Nested Mass and MunCnt_Spread for 1-way, reduced 2-way and reduced 3-way models

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	Agent	Season	Time	HOR	MunCnt_Spread	Mass	PCAS	limits
1	T	F	12	0	1	1	0.746	(0.710, 0.780)
2	T	F	12	0	1	1.5714	0.763	(0.732, 0.793)
3	T	F	12	0	1	2	0.788	(0.756, 0.819)
4	T	F	12	0	2	1	0.802	(0.771, 0.832)
5	T	F	12	0	2	1.5714	0.818	(0.789, 0.846)
6	T	F	12	0	2	2	0.841	(0.812, 0.867)

1-way Model, Highlighted Prediction is 0.802 ± **0.030**
Based on fitting 36 trials

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	Agent	Season	Time	HOR	MunCnt_Spread	Mass	PCAS	limits
1	T	F	12	0	1	1	0.724	(0.715, 0.733)
2	T	F	12	0	1	1.5714	0.772	(0.763, 0.780)
3	T	F	12	0	1	2	0.795	(0.787, 0.803)
4	T	F	12	0	2	1	0.803	(0.795, 0.811)
5	T	F	12	0	2	1.5714	0.835	(0.828, 0.843)
6	T	F	12	0	2	2	0.851	(0.844, 0.858)

2-way Model, Highlighted Prediction is 0.803 ± **0.008**
Based on fitting 108 trials

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	Agent	Season	Time	HOR	MunCnt_Spread	Mass	PCAS	limits
1	T	F	12	0	1	1	0.730	(0.730, 0.730)
2	T	F	12	0	1	1.5714	0.772	(0.772, 0.772)
3	T	F	12	0	1	2	0.793	(0.793, 0.793)
4	T	F	12	0	2	1	0.802	(0.802, 0.802)
5	T	F	12	0	2	1.5714	0.837	(0.837, 0.837)
6	T	F	12	0	2	2	0.854	(0.854, 0.854)

3-way Model, Highlighted Prediction is 0.802 ± **0.000**
Based on fitting 324 trials

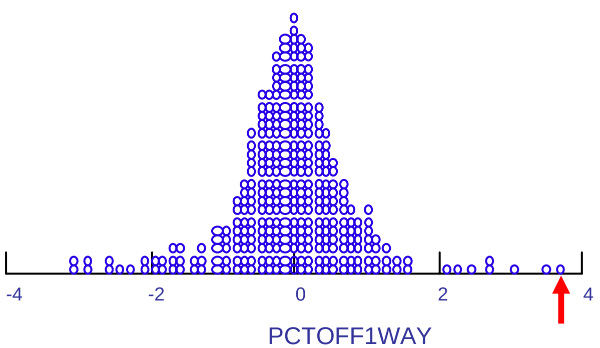
Percent Off Target for 324 PCAS Checkpoint Predictions with 1-Way, 2-Way and 3-Way Models "How Good is Good Enough?"

1-way Model
Fit to 36 Trials in
Stage 1 Design

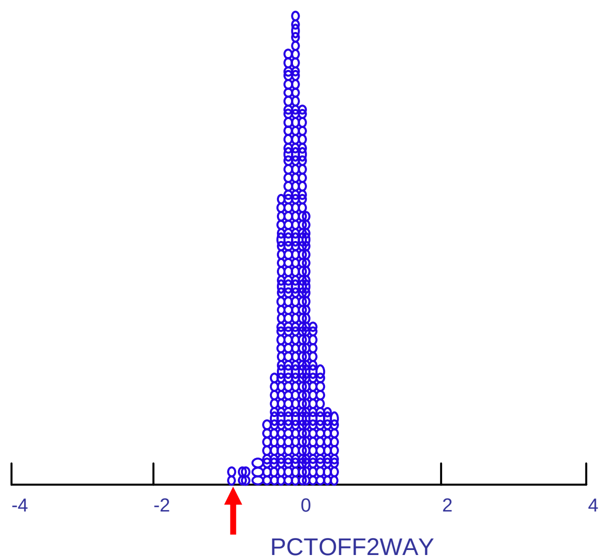
Reduced 2-way Model
Fit to 36 + 72 Trials in
Stage 2 Design

Reduced 3-way Model
Fit to 36 + 72 + 216 Trials in
Stage 3 Design

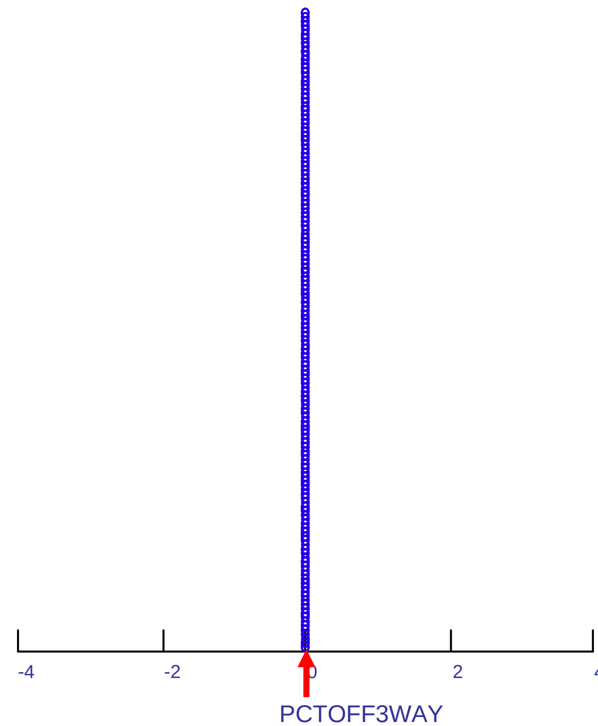
Common Scale range for plots is from -4% to 4%



Worst Case = 3.7%
Half of Cases < 0.37%



Worst Case = -0.93%
Half of Cases < 0.11%



Worst Case = 0.008%
Half of Cases < 0.001%

Seminal Paper on "Smoothing*" DOE for Computer Experiments

- **Sacks, J., Welch, W.J., Mitchell, T.J. and Wynn, H.P. (1989). "Design and Analysis of Computer Experiments." *Statistical Science* 4. 409-423**
  - First textbook appeared in 2003 and has the same name
  - A good source for up-to-date information is the Simulation Experiments & Efficient Designs (SEED) Center for Data Farming at http://harvest.nps.edu

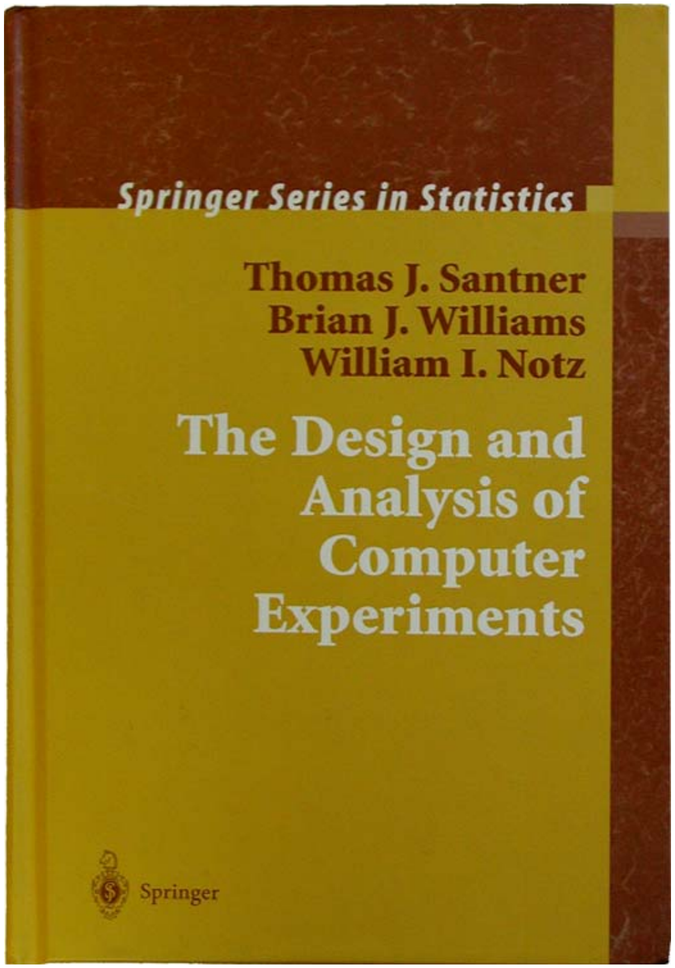
*Smoothing is an alternate name sometimes used for designs for computer experiments because it is a good description of the end result of the analysis. Another name that sometimes appears is "space-filling" designs because trials are spread somewhat uniformly throughout the test volume.

How are Smoothing Designs Different?

- **From the traditional experimental design point of view the Smoothing designs – for the same number of trials – do not enclose as large a volume of the design space. This is intentional.**
- **Rather than emphasizing high leverage trials ("corners") for a simple polynomial model, these designs "spread" their trials more uniformly through the space to better capture the local complexities of the simulation model.**
- **Analysis employs "Kriging" method originally developed for geo-spatial regression**

Optimization of Modeled Industrial Process Using Computer Experiments

- Data is generated by a simulation consisting of a *series* of physical/chemical models each feeding its result into the next.
- Industrial examples include:
  - Chemical plant
  - Aircraft engines
  - Deep ocean oil production
  - Semiconductor fabrication line
  - Aluminum can extruder
    - Ran 51 "designed" simulation trials, analyzed data, determined optimal factor settings, checked optimum with a simulation trial (they agreed), built 1 real machine for $500,000 and made real cans – the performance was "dead on"
- DoD examples include M&S like the ECBC Chem-Bio Sim Suite, SOES Smoke Model, etc.



C.3 Examples

The following examples demonstrate many possible uses of PErK. The responses for these examples are based on the *Branin function*. The Branin function is the real-valued function of two variables

$$y_{\mathcal{B}}(x_1, x_2) = \left(x_2 - \frac{5.1}{4\pi^2}\,x_1^2 + \frac{5}{\pi}\,x_1 - 6\right)^2 + 10\left(1 - \frac{1}{8\pi}\right)\cos(x_1) + 10$$

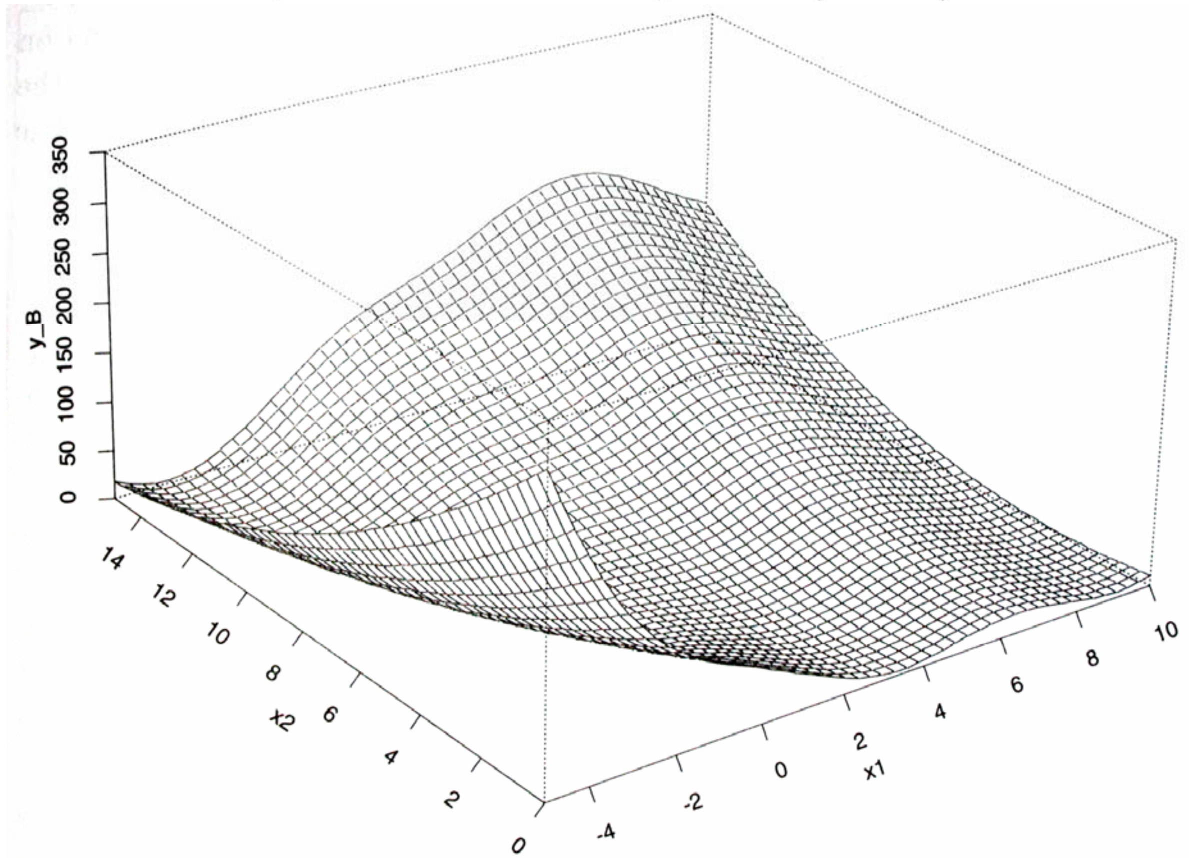
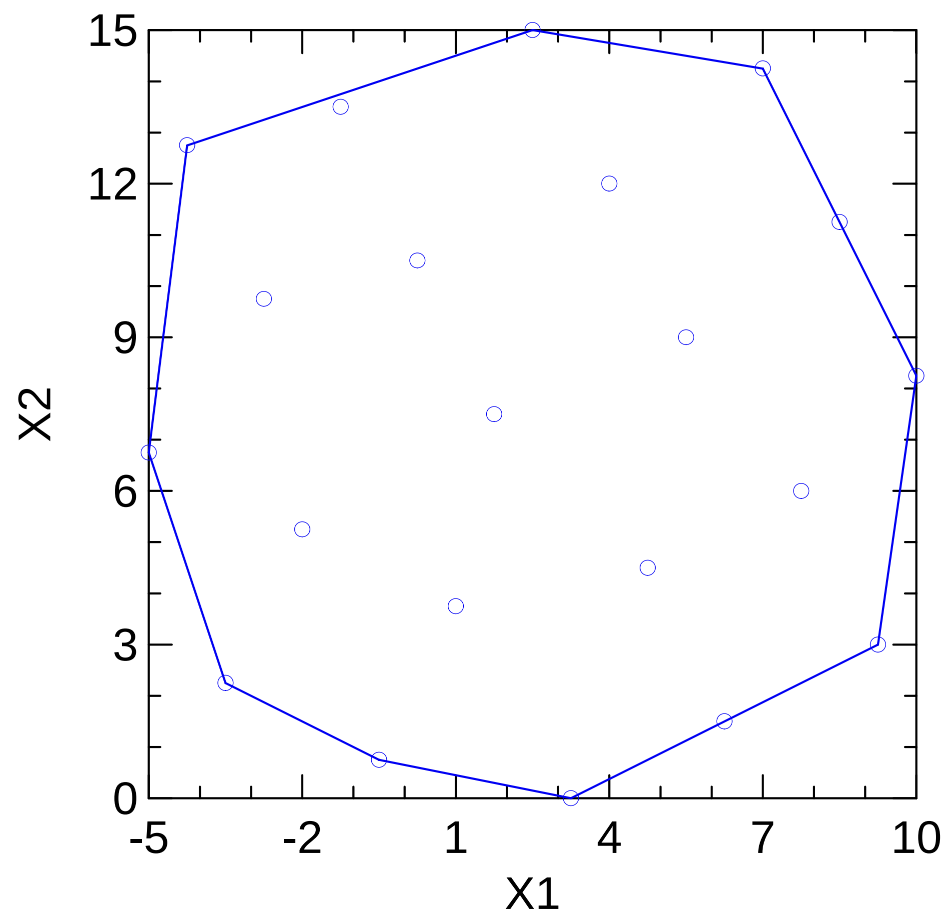


FIGURE C.1. The Branin function on $[-5, 10] \times [0, 15]$

Example Latin Hypercube Design and Data Calculated with Branin Function

Trial	X1	X2	Y
1	7.75	6	35.80951
2	1	3.75	14.86287
3	10	8.25	31.41880
4	4.75	4.5	19.87899
5	2.5	15	141.88566
6	-3.5	2.25	99.43335
7	3.25	0	3.88973
8	-5	6.75	97.47380
9	-4.25	12.75	6.27060
10	6.25	1.5	19.85914
11	8.5	11.25	95.50587
12	7	14.25	181.74214
13	-0.5	0.75	49.39445
14	-2	5.25	23.13762
15	0.25	10.5	43.09524
16	9.25	3	2.82392
17	-2.75	9.75	3.61474
18	5.5	9	75.79100
19	4	12	104.11175
20	-1.25	13.5	43.33586
21	1.75	7.5	23.39797



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Trial	X1	X2	Y
1	7.75	6	35.80951
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19	4	12	104.11175
20	-1.25	13.5	43.33586
21	1.75	7.5	23.39797

Plot from textbook of Branin Function

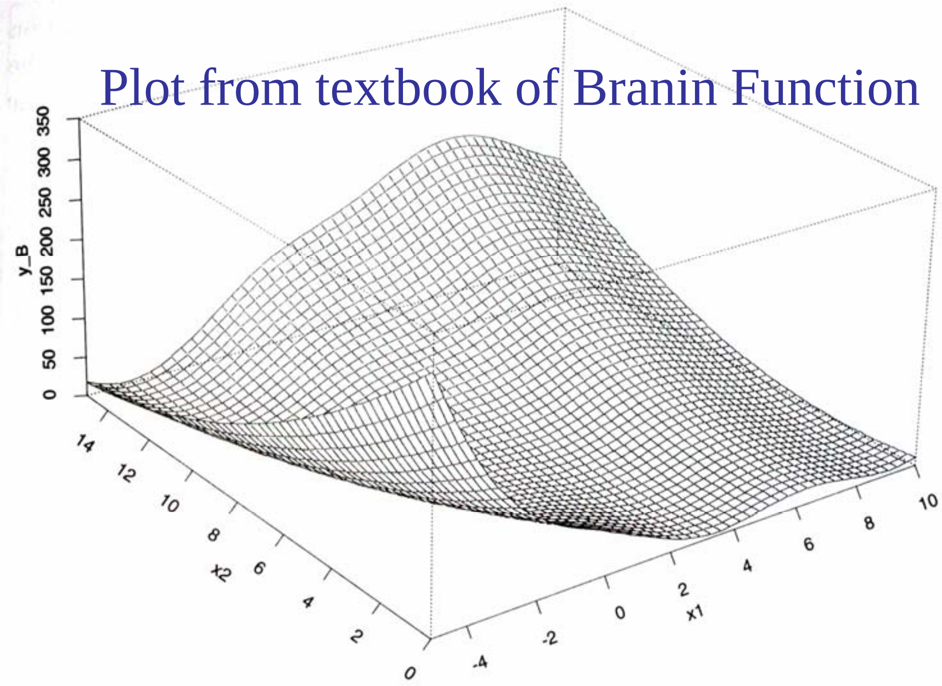
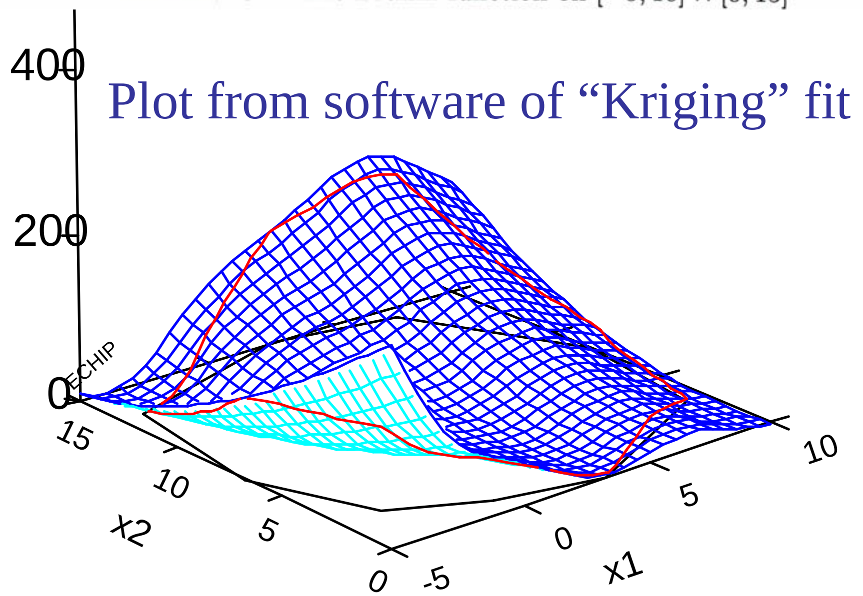


FIGURE C.1. The Branin function on $[-5, 10] \times [0, 15]$

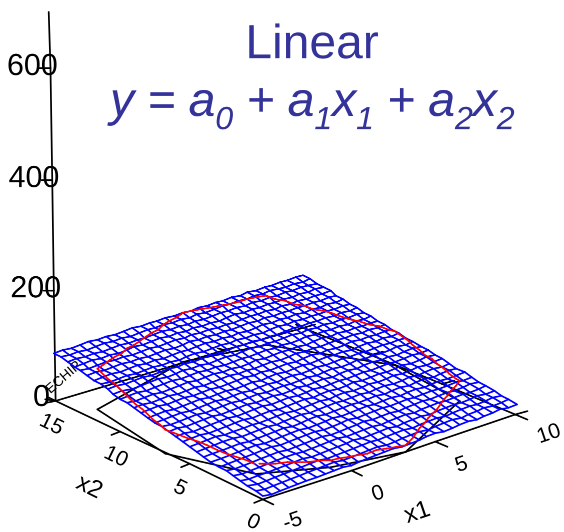
Plot from software of “Kriging” fit



Comparing Surfaces for Increasingly Complex Polynomials Fit to Data from the Branin Function

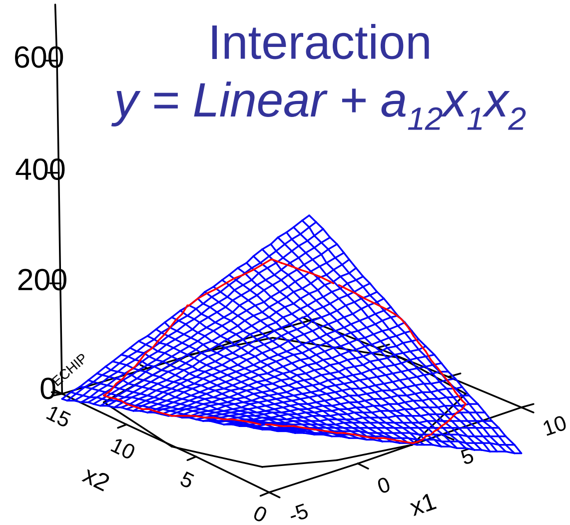
Linear

$y = a_0 + a_1x_1 + a_2x_2$



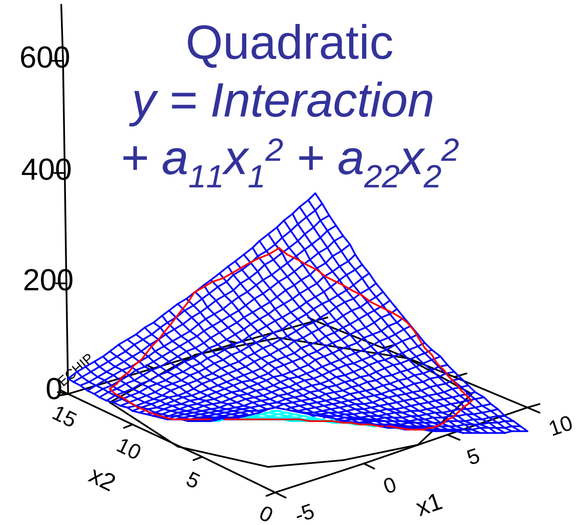
Interaction

$y = Linear + a_{12}x_1x_2$



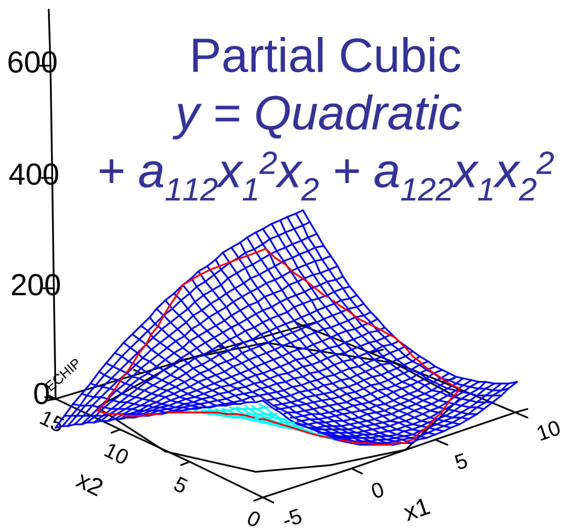
Quadratic

$y = Interaction + a_{11}x_1^2 + a_{22}x_2^2$



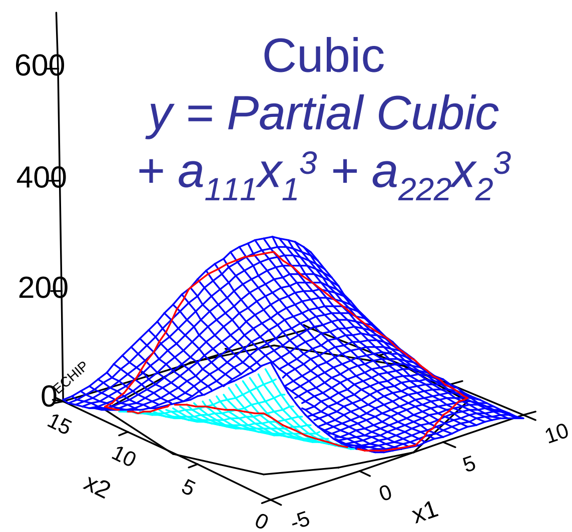
Partial Cubic

$y = Quadratic + a_{112}x_1^2x_2 + a_{122}x_1x_2^2$

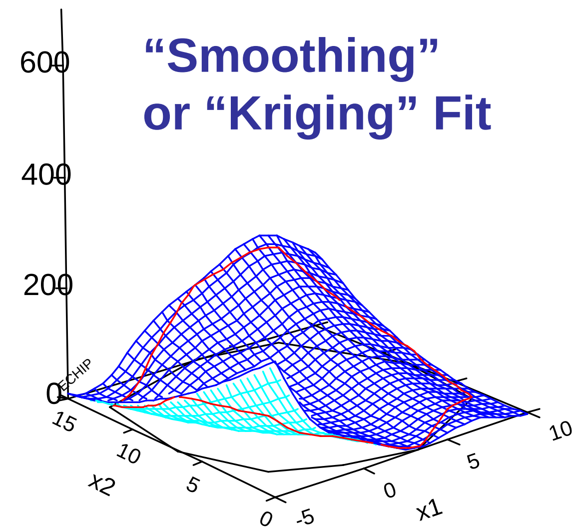


Cubic

$y = Partial\ Cubic + a_{111}x_1^3 + a_{222}x_2^3$



“Smoothing” or “Kriging” Fit



The full *cubic* model appears to closely approximate the Branin function, but still cannot represent the ripples seen in the fit using Kriging method.

CB Sim Suite Smoothing DOE Example with 10 Variables

- **Branin function example is trivial. With 2 control variables the full cubic model has 10 terms.**
- **The following example has 10 control variables. (Full cubic model has 166 terms!)**
- **Three different Smoothing designs are used:**

1. 17-trial Latin Hypercube (LHC) design
2. 33-trial Nearly Orthogonal Latin Hypercube (NOLH) design (see SEED web site at http://harvest.nps.edu)
3. 50-trial Orthogonal Array (OA) design.

- **Smoothing design trials combine in such a way as to fall into 5 of 6 Pasquill Atmospheric Stability regions within the VLSTRACK model**

Pasquill Atmospheric Stability Classes & Meteorological Conditions That Define Them

Stability Class	Definition
A	very unstable
B	unstable
C	slightly unstable
D	neutral
E	slightly stable
F	stable

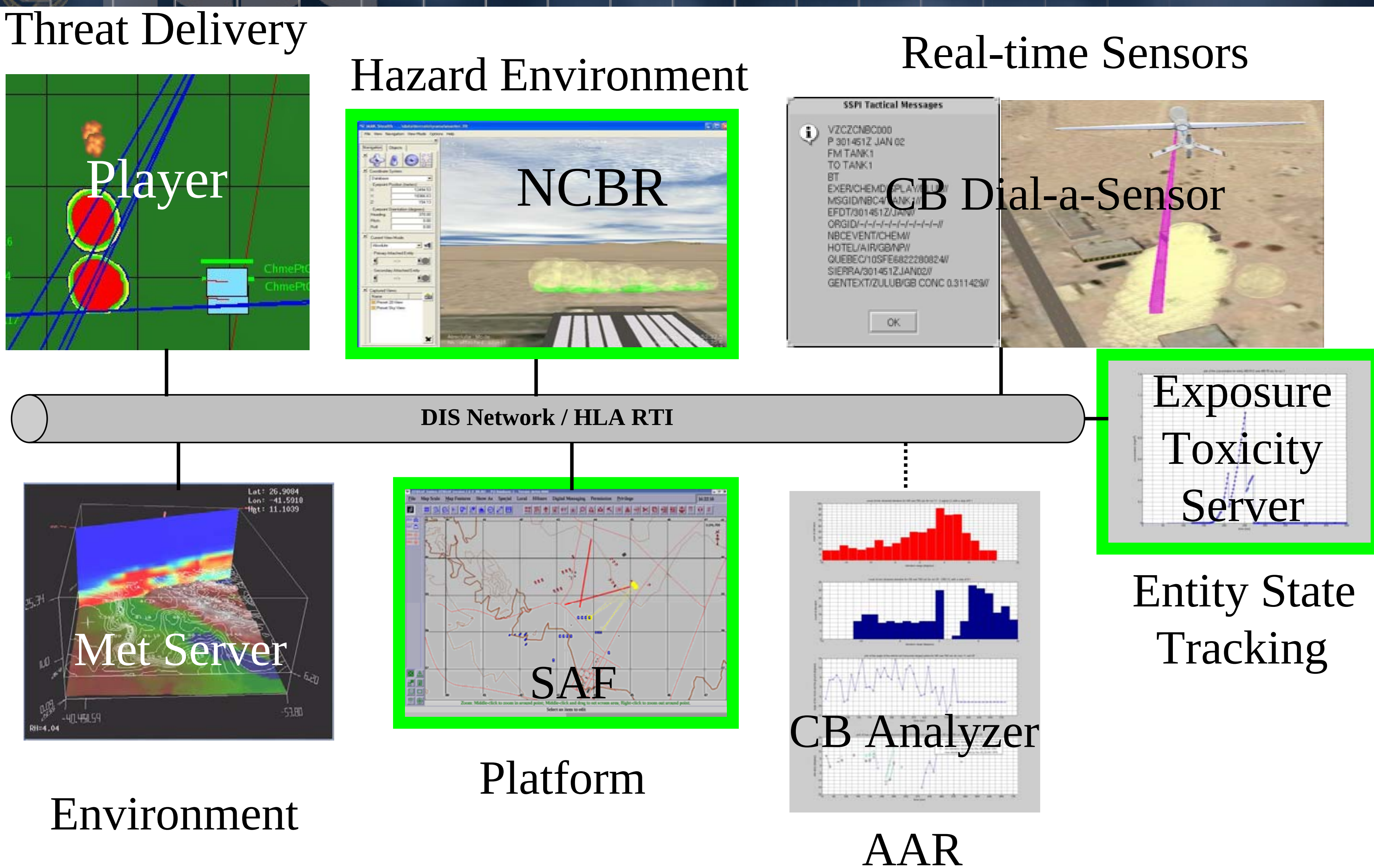
Key point is that VLSTRACK models each class a bit differently and we want to create a single meta-model of all classes together

Surface Wind Speed		Daytime Incoming Solar Radiation			Nighttime Cloud Cover	
m/s	mi/hr	Strong	Moderate	Slight	> 50%	< 50%
< 2	< 5	A	A - B	B	E	F
2 to 3	5 to 7	A - B	B	C	E	F
3 to 5	7 to 11	B	B - C	C	D	E
5 to 6	11 to 13	C	C - D	D	D	D
> 6	> 13	C	D	D	D	D
Note: Class D applies to heavily overcast skies, at any windspeed day or night						

TABLES SOURCE : http://en.wikipedia.org/wiki/Air_pollution_dispersion_terminology#_note-7#_note-7

ORIGINAL SOURCE: Pasquill, F. (1961). *The estimation of the dispersion of windborne material*, The Meteorological Magazine, vol 90, No. 1063, pp 33-49.

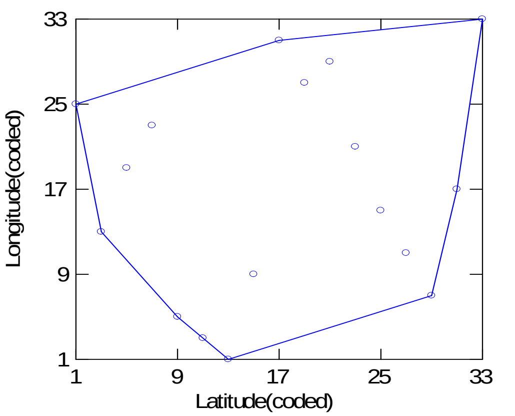
CB Simulation Suite Architecture



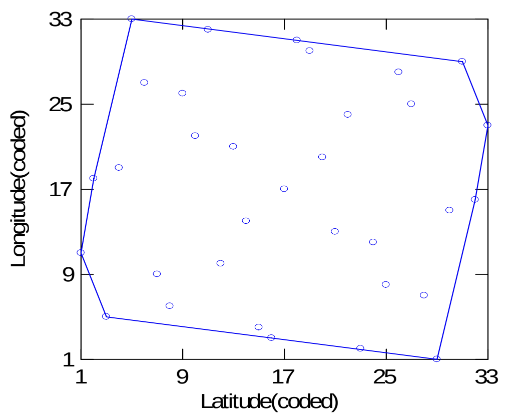
CB Sim Suite is a set of distributed simulation tools designed to represent all aspects of CB passive defense on the tactical battle field for application to analysis, testing, and training.

Projections in 2-D for 3 Different 10-Variable “Smoothing” Designs of Size 17, 33 & 50 Trials

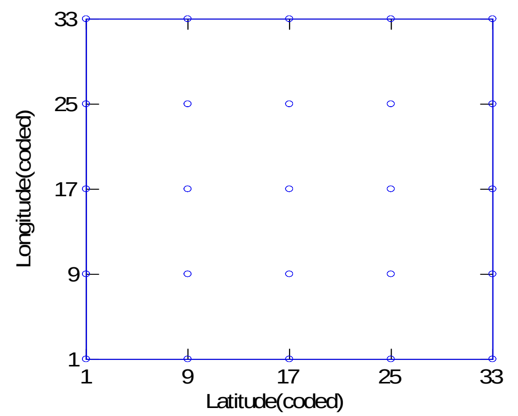
17-trial
Latin HyperCube (LHC)



33-trial
Nearly Orthogonal
Latin Hypercube (NOLH)



50-trial
Orthogonal Array (OA)



Trial #	Second (0 -61)	Minute (0 - 59)	Hour (0 - 23)	Day (1 - 31)	Month (0 - 11) since Jan.	Year (since 1900)	Pasquill Constant	Temp (degrees C)	Wind Speed (m/s)	Wind Direction (degrees from north)	Humidity (percentage)	Cloud Cover (decimal percentage)	Amount of Agent (kg)	Duration (seconds)	Trial #	Latitude (coded)
34	0	40	17	16	2	107	0	27	2.6	268	60	0.92	200	13.34	34	3
35	0	40	18	16	2	107	0	31	5.3	278	70	0.26	80	56.23	35	21
36	0	40	19	16	2	107	0	11	3.8	280	30	0.38	180	42.17	36	5
37	0	40	20	16	2	107	0	7	5.6	254	50	0.62	60	4.22	37	15
38	0	40	21	16	2	107	0	23	2.9	282	55	0.32	100	7.50	38	17
39	0	40	22	16	2	107	0	25	4.1	286	15	0.14	40	23.71	39	9
40	0	40	23	16	2	107	0	21	1.4	266	35	0.74	280	31.62	40	19
41	0	40	0	17	2	107	0	19	4.4	262	85	0.08	160	5.62	41	27
42	0	40	1	17	2	107	0	13	3.2	260	10	0.02	140	10.00	42	29
43	0	40	2	17	2	107	0	17	4.7	272	45	0.98	300	74.99	43	23
44	0	40	3	17	2	107	0	5	2.3	264	90	0.8	260	1.78	44	33
45	0	40	4	17	2	107	0	35	1.7	256	65	0.44	240	100.00	45	11
46	0	40	5	17	2	107	0	15	3.5	270	25	0.68	120	1.33	46	7
47	0	40	6	17	2	107	0	9	6.2	284	75	0.2	340	1.00	47	31
48	0	40	7	17	2	107	0	37	5.9	276	40	0.5	360	2.37	48	25
49	0	40	8	17	2	107	0	29	5	274	20	0.56	220	17.78	49	13
50	0	40	9	17	2	107	0	33	2	258	80	0.86	320	3.16	50	1

Trial #	Second (0 -61)	Minute (0 - 59)	Hour (0 - 23)	Day (1 - 31)	Month (0 - 11) since Jan.	Year (since 1900)	Pasquill Constant	Temp (degrees C)	Wind Speed (m/s)	Wind Direction (degrees from north)	Humidity (percentage)	Cloud Cover (decimal percentage)	Amount of Agent (kg)	Duration (seconds)	Trial #	Latitude (coded)
1	0	40	17	16	2	107	0	34	4.1	280	20	0.38	140	11.5	1	1
2	0	10	18	16	2	107	0	7	4.7	277	55	0.77	310	1.78	2	32
3	0	40	18	16	2	107	0	36	3.95	279	35	0.29	230	7.50	3	31
4	0	10	19	16	2	107	0	5	5.6	274	52.5	0.8	120	23.7	4	4
5	0	40	19	16	2	107	0	23	1.85	281	87.5	0.41	130	86.6	5	23
6	0	10	20	16	2	107	0	18	4.4	258	77.5	0.44	60	3.65	6	25
7	0	40	20	16	2	107	0	17	3.35	254	25	0.11	180	4.87	7	7
8	0	10	21	16	2	107	0	14	3.05	256	30	0.05	210	15.4	8	26
9	0	40	21	16	2	107	0	16	4.85	264	72.5	0.47	330	17.8	9	6
10	0	10	22	16	2	107	0	30	2.6	255	62.5	0.92	320	48.7	10	21
11	0	40	22	16	2	107	0	22	1.55	278	90	0.35	240	1.54	11	5
12	0	10	23	16	2	107	0	29	5.15	269	32.5	0.68	360	42.2	12	14
13	0	40	23	16	2	107	0	31	2.15	257	60	0.98	150	3.16	13	10
14	0	10	0	17	2	107	0	32	5.3	268	42.5	0.86	50	2.74	14	22
15	0	40	0	17	2	107	0	9	1.4	273	15	0.83	100	75.0	15	19
16	0	10	1	17	2	107	0	15	1.7	275	17.5	0.74	290	1.00	16	16
17	0	40	1	17	2	107	0	21	3.8	270	50	0.5	200	10.0	17	17
18	0	10	2	17	2	107	0	27	5.9	265	82.5	0.26	110	100.0	18	18
19	0	40	2	17	2	107	0	33	6.2	267	85	0.17	300	1.33	19	15
20	0	10	3	17	2	107	0	10	2.3	272	57.5	0.14	350	36.5	20	12
21	0	40	3	17	2	107	0	11	5.45	283	40	0.02	250	31.6	21	24
22	0	10	4	17	2	107	0	13	2.45	271	67.5	0.32	40	2.37	22	20
23	0	40	4	17	2	107	0	20	6.05	262	10	0.65	160	64.9	23	29
24	0	10	5	17	2	107	0	12	5	285	37.5	0.08	80	2.05	24	13
25	0	40	5	17	2	107	0	26	2.75	276	27.5	0.53	70	5.62	25	28
26	0	10	6	17	2	107	0	28	4.55	284	70	0.95	190	6.49	26	8
27	0	40	6	17	2	107	0	25	4.25	286	75	0.89	220	20.5	27	27
28	0	10	7	17	2	107	0	24	3.2	282	22.5	0.56	340	27.4	28	9
29	0	40	7	17	2	107	0	19	5.75	259	12.5	0.59	270	1.15	29	11
30	0	10	8	17	2	107	0	37	2	266	47.5	0.2	280	4.22	30	30
31	0	40	8	17	2	107	0	6	3.65	261	65	0.71	170	13.3	31	3
32	0	10	9	17	2	107	0	35	2.9	263	45	0.23	90	56.2	32	2
33	0	40	9	17	2	107	0	8	3.5	260	80	0.62	260	8.66	33	33

Trial #	Second (0 -61)	Minute (0 - 59)	Hour (0 - 23)	Day (1 - 31)	Month (0 - 11) since Jan.	Year (since 1900)	Pasquill Constant	Temp (degrees C)	Wind Speed (m/s)	Wind Direction (degrees from north)	Humidity (percentage)	Cloud Cover (decimal percentage)	Amount of Agent (kg)	Duration (seconds)	Trial #	Latitude (coded)
51	0	40	17	16	2	107	0	5	1.4	254	10	0.02	40	1.00	51	1
52	0	40	17	16	2	107	0	13	2.6	262	30	0.26	200	31.62	52	33
53	0	40	17	16	2	107	0	21	3.8	270	50	0.98	120	31.62	53	1
54	0	40	17	16	2	107	0	29	5	278	70	0.98	200	1.00	54	25
55	0	40	17	16	2	107	0	37	6.2	286	90	0.26	40	100.00	55	25
56	0	40	17	16	2	107	0	13	5	270	90	0.02	280	10.00	56	17
57	0	40	17	16	2	107	0	21	6.2	278	10	0.74	360	3.16	57	33
58	0	40	17	16	2	107	0	29	1.4	286	30	0.5	120	3.16	58	17
59	0	40	17	16	2	107	0	37	2.6	254	50	0.5	360	10.00	59	9
60	0	40	17	16	2	107	0	5	3.8	262	70	0.74	280	100.00	60	9
61	0	40	21	16	2	107	0	13	3.8	278	90	0.26	120	3.16	61	9
62	0	40	21	16	2	107	0	21	5	286	10	0.5	280	100.00	62	1
63	0	40	21	16	2	107	0	29	6.2	254	30	0.02	200	100.00	63	9
64	0	40	21	16	2	107	0	37	1.4	262	50	0.02	280	3.16	64	33
65	0	40	21	16	2	107	0	5	2.6	270	70	0.5	120	1.00	65	33
66	0	40	21	16	2	107	0	21	1.4	254	70	0.26	360	31.62	66	25
67	0	40	21	16	2	107	0	29	2.6	262	90	0.98	40	10.00	67	1
68	0	40	21	16	2	107	0	37	3.8	270	10	0.74	200	10.00	68	25
69	0	40	21	16	2	107	0	5	5	278	30	0.74	40	31.62	69	17
70	0	40	21	16	2	107	0	13	6.2	286	50	0.98	360	1.00	70	17
71	0	40	1	17	2	107	0	21	6.2	262	70	0.5	200	10.00	71	17
72	0	40	1	17	2	107	0	29	1.4	270	90	0.74	360	1.00	72	9
73	0	40	1	17	2	107	0	37	2.6	278	10	0.26	280	1.00	73	17
74	0	40	1	17	2	107	0	5	3.8	286	30	0.26	360	10.00	74	1
75	0	40	1	17	2	107	0	13	5	254	50	0.74	200	3.16	75	1
76	0	40	1	17	2	107	0	29	3.8	278	50	0.5	40	100.00	76	33
77	0	40	1	17	2	107	0	37	5	286	70	0.02	120	31.62	77	9
78	0	40	1	17	2	107	0	5	6.2	254	90	0.98	280	31.62	78	33
79	0	40	1	17	2	107	0	13	1.4	262	10	0.98	120	100.00	79	25
80	0	40	1	17	2	107	0	21	2.6	270	30	0.02	40	3.16	80	25
81	0	40	5	17	2	107	0	29	2.6	286	50	0.74	280	31.62	81	25
82	0	40	5	17	2	107	0	37	3.8	254	70	0.98	40	3.16	82	17
83	0	40	5	17	2	107	0	5	5	262	90	0.5	360	3.16	83	25
84	0	40	5	17	2	107	0	13	6.2	270	10	0.5	40	31.62	84	9
85	0	40	5	17	2	107	0	21	1.4	278	30	0.98	280	10.00	85	9
86	0	40	5	17	2	107	0	37	6.2	262	30	0.74	120	1.00	86	1
87	0	40	5	17	2	107	0	5	1.4	270	50	0.26	200	100.00	87	17
88	0	40	5	17	2	107	0	13	2.6	278	70	0.02	360	100.00	88	1
89	0	40	5	17	2	107	0	21	3.8	286	90	0.02	200	1.00	89	33
90	0	40	5	17	2	107	0	29	5	254	10	0.26	120	10.00	90	33
91	0	40	9	17	2	107	0	37	5	270	30	0.98	360	100.00	91	33
92	0	40	9	17	2	107	0	5	6.2	278	50	0.02	120	10.00	92	25
93	0	40	9	17	2	107	0	13	1.4	286	70	0.74	40	10.00	93	33
94	0	40	9	17	2	107	0	21	2.6	254	90	0.74	120	100.00	94	17
95	0	40	9	17	2	107	0	29	3.8	262	10	0.02	360	31.62	95	17
96	0	40	9	17	2	107	0	5	2.6	286	10	0.98	200	3.16	96	9
97	0	40	9	17	2	107	0	13	3.8	254	30	0.5	280	1.00	97	25
98	0	40	9	17	2	107	0	21	5	262	50	0.26	40	1.00	98	9
99	0	40	9	17	2	107	0	29	6.2	270	70	0.26	280	3.16	99	1
100	0	40	9	17	2	107	0	37	1.4	278	90	0.5	200	31.62	100	1

UNCLASSIFIED/UNLIMITED

50-trial Orthogonal Array with 5 Levels per Variable

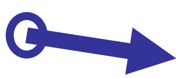
C:\DOCUME~1\THOMAS~1.DON\LOCALS~1\Temp\DESIGN.ECH

TRIAL	time_wrt_sunset	Temp	Wind_speed	Wind_direction	Humidity	Cloud_Cover	Amount_Agent	Log(duration)	Latitude(coded)	Longitude(coded)
51	-120	5	1.4	254	10	0.02	40	0	1	1
52	-120	13	2.6	262	30	0.26	200	1.5	33	1
53	-120	21	3.8	270	50	0.98	120	1.5	1	17
54	-120	29	5	278	70	0.98	200	0	25	9
55	-120	37	6.2	286	90	0.26	40	2	25	17
56	-120	13	5	270	90	0.02	280	1	17	25
57	-120	21	6.2	278	10	0.74	360	0.5	33	25
58	-120	29	1.4	286	30	0.5	120	0.5	17	33
59	-120	37	2.6	254	50	0.5	360	1	9	9
60	-120	5	3.8	262	70	0.74	280	2	9	33
61	120	13	3.8	278	90	0.26	120	0.5	9	9
62	120	21	5	286	10	0.5	280	2	1	9
63	120	29	6.2	254	30	0.02	200	2	9	25
64	120	37	1.4	262	50	0.02	280	0.5	33	17
65	120	5	2.6	270	70	0.5	120	0	33	25
66	120	21	1.4	254	70	0.26	360	1.5	25	33
67	120	29	2.6	262	90	0.98	40	1	1	33

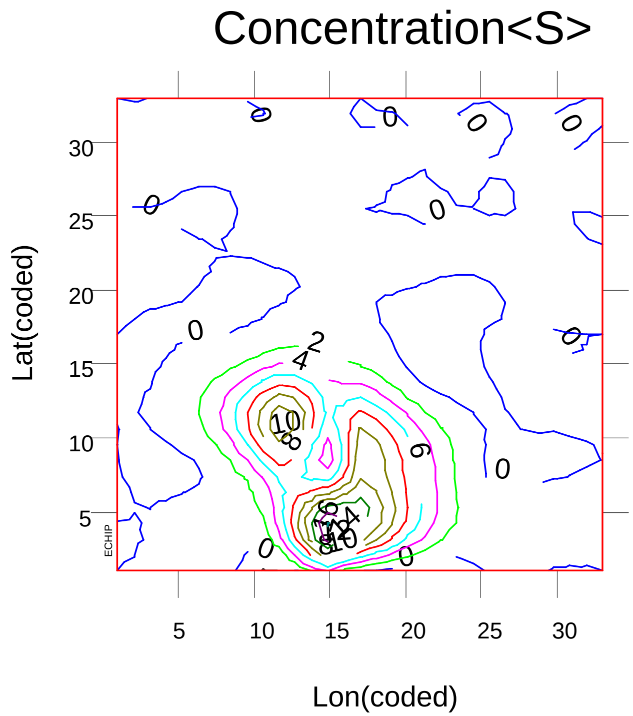
Showing first 17 of 50 trials in one "space-filling" design out of 5^{10} = 9,765,625 possible combinations of variable settings

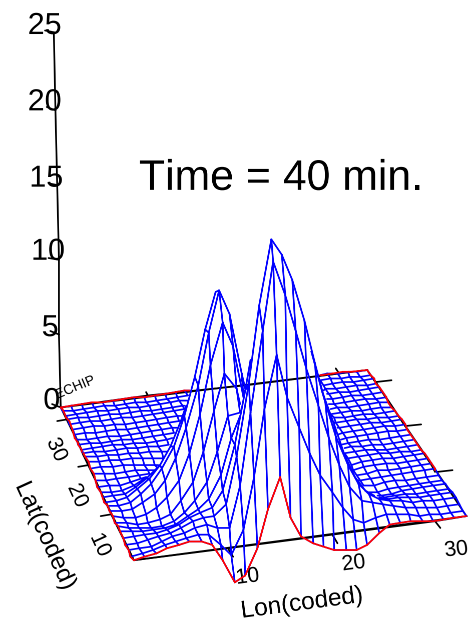
Kriging Analysis of a Single Simulation – Concentration vs. Latitude, Longitude & Time

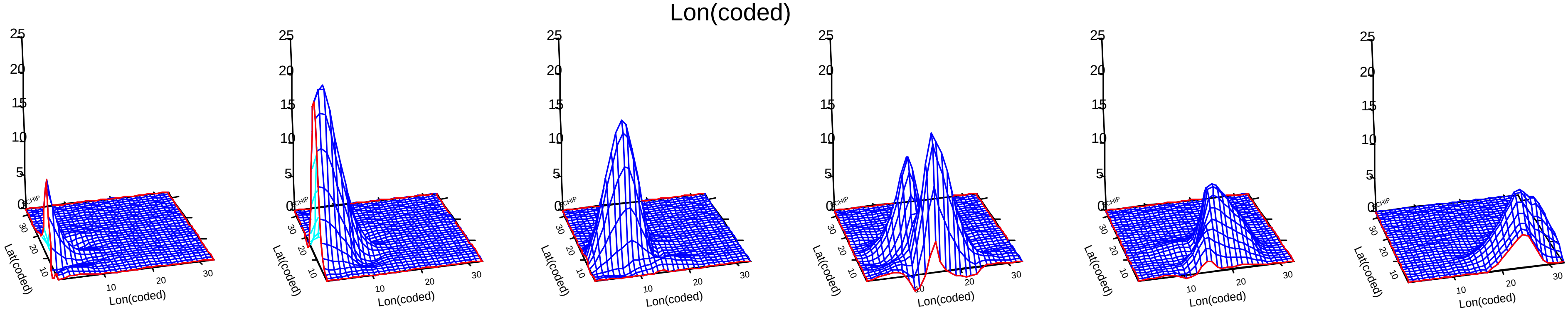
Cloud release point is 10 km west of 10 km X 10 km grid of 72 identical entities



Wind speed is 5.3 m/s
Wind direction is 278° from north



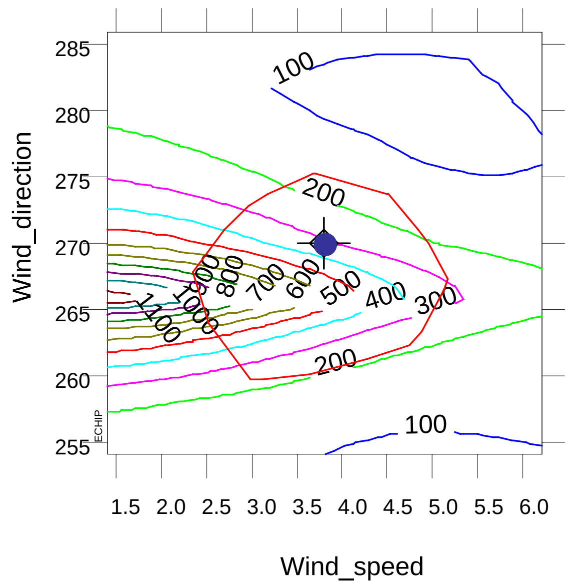




28 min. | 32 min. | 36 min. | 40 min. | 44 min. | 48 min.

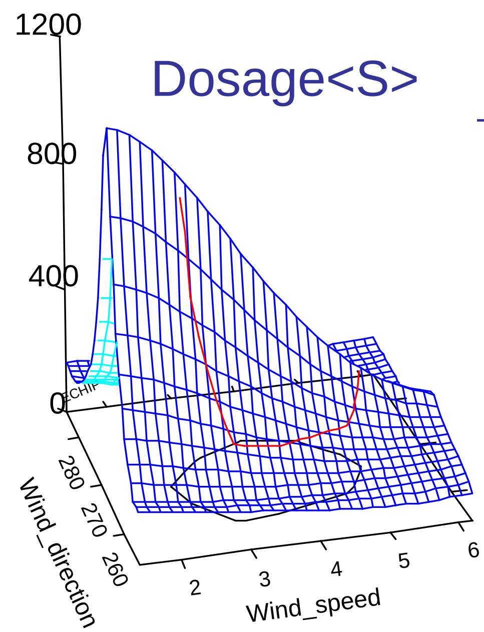
Kriging Analysis of 17 LHC Simulations Using 17 Observations Max Dosage vs. 8 Variables

Dosage<S>

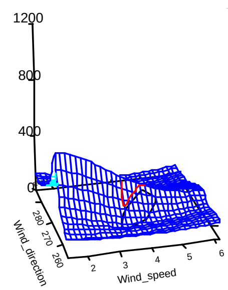
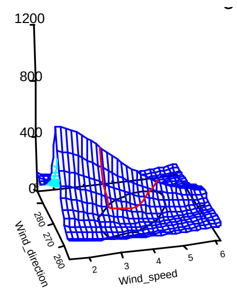
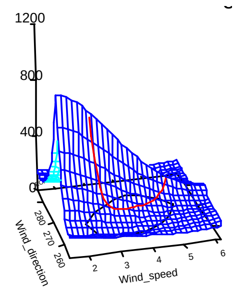
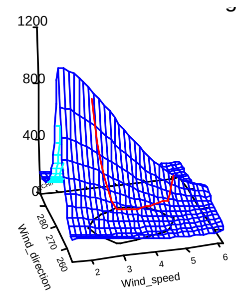
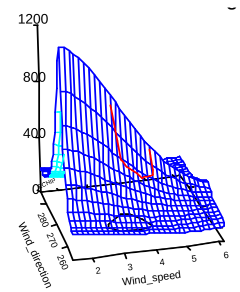
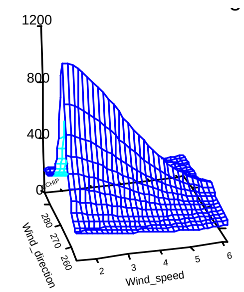


time_wrt_sunset = 360.0
Temp = 21.0
Humidity = 50.0
Cloud_Cover = 0.620
Amount_Agent = 200.0
Log(duration) = 1.0

Wind_spe=3.80 Value 311.82	Wind_dir=270.00



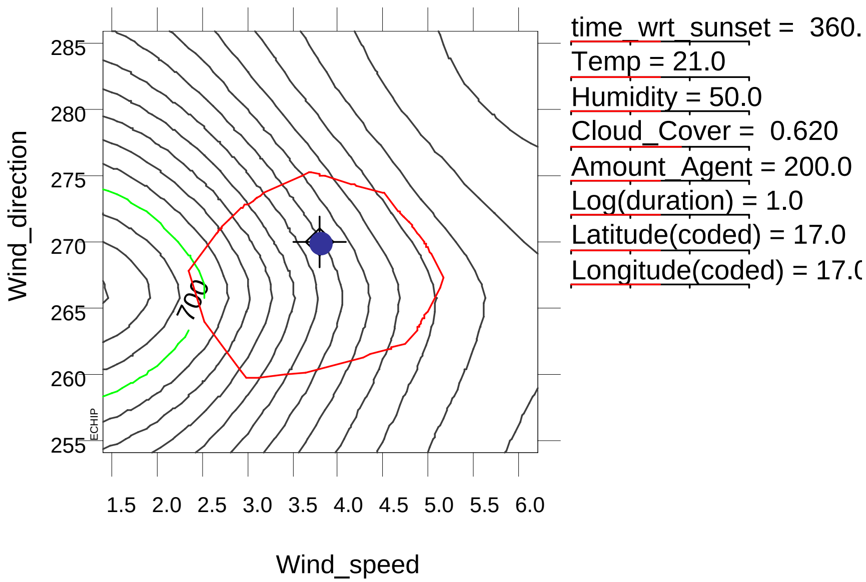
Time wrt Sunset = 360
Temperature = 21
Humidity = 50
Cloud Cover = 0.62
Amount_Agent = 200
Log_{10}(Duration) = 1

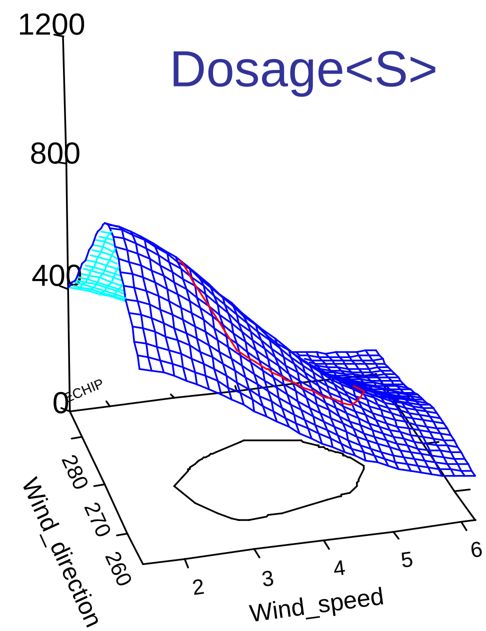
Cloud Cover = 0.26 0.38 0.50 0.62 0.74 0.86

Kriging Analysis of 17 LHC Simulations Using 1209 Observations = 17 X 72 – 15 Max Dosage vs. 10 Variables

Dosage<S>

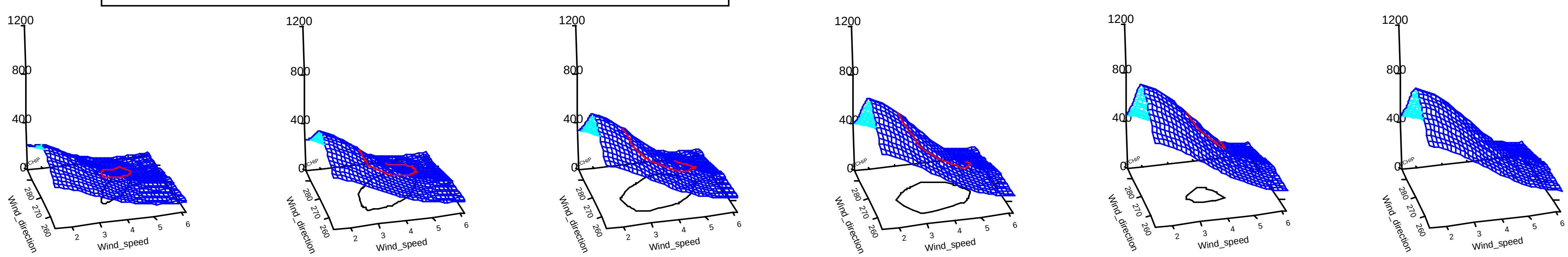


Wind_spe=3.80	Wind_dir=270.00
Value 404.61	



Dosage<S>

Time wrt Sunset = 360
Temperature = 21
Humidity = 50
Cloud Cover = 0.62
Amount_Agent = 200
Log_{10}(Duration) = 1
Latitude = 17
Longitude = 17



Cloud Cover = 0.26 0.38 0.50 0.62 0.74 0.86

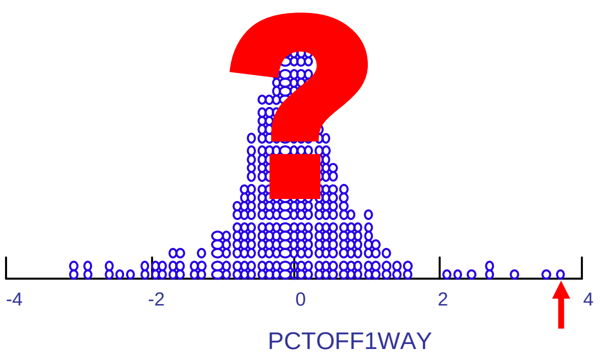
In Future Will Show % Off Target for 200 Checkpoint Predictions with Various Smoothing Designs "Suspect - Never Get Something for Nothing"

Kriging Model
Fit to 17 Trials in
LHC

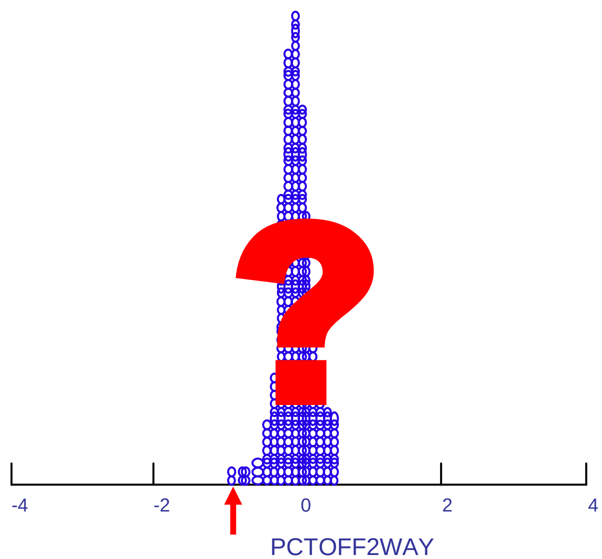
Kriging Model
Fit to 17 +33 Trials in
LHC + NOLH

Kriging Model
Fit to 17 + 33 + 50 Trials in
LHC + NOLH + OA

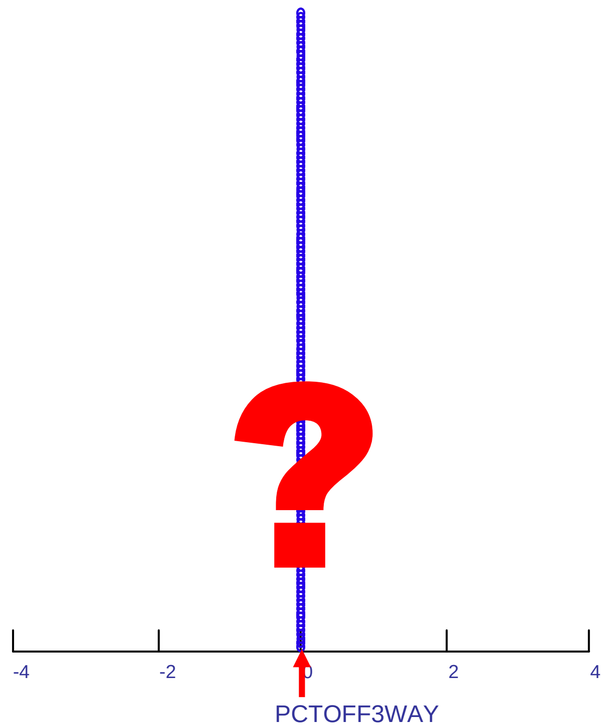
Common Scale range for plots is from -4% to 4%



Worst Case = ?%
Half of Cases < ?%



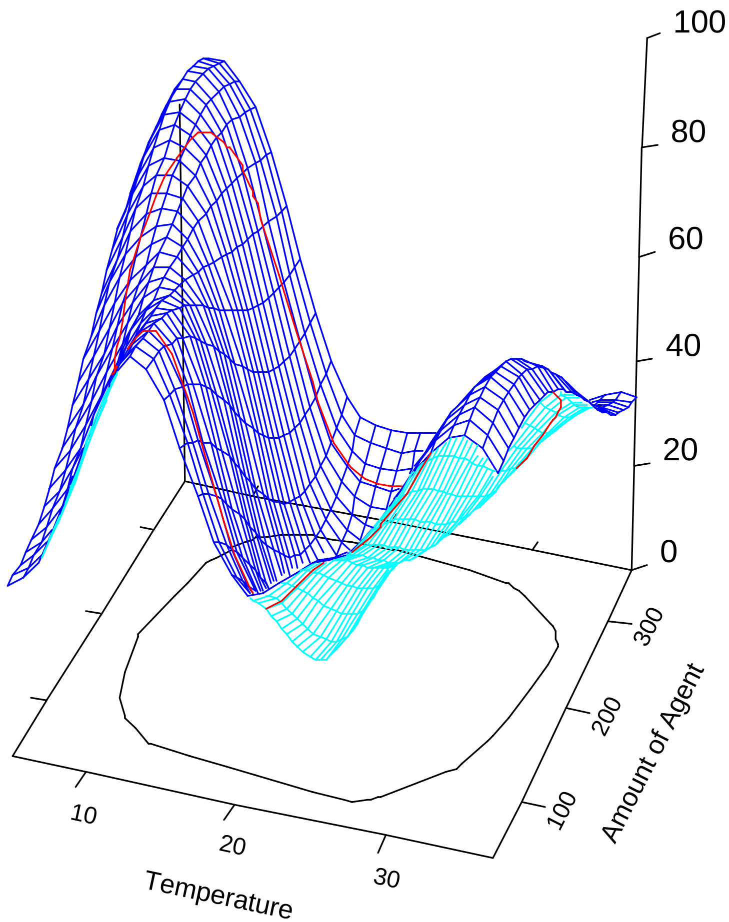
Worst Case = ?%
Half of Cases < ?%



Worst Case = ?%
Half of Cases < ?%

Kriging Analysis of Random Data!

10-Variable Meta-Model Predicting Concentration



Off-Axis Variable Settings

Time wrt Sunset = 360
Wind Speed = 3.8
Wind Direction = 270
Humidity = 50
Cloud Cover = 0.50
Log_{10}(Duration) = 1.0
Latitude (coded) = 17
Longitude (coded) = 17

NOTE: This is a plot of Kriging regression of the 100 integers between 0 and 99 randomly assigned to 100 smoothing design trials.
The “noise” has been fit perfectly!
This is why one should only use this technique with non-random data!

ECBC

Summary

- Demonstrated how Design of Experiments (DOE) can be used to sequentially run groups of simulation trials to obtain better and better meta-models of the simulation model
- When control variables are all continuous and response variable is NON-stochastic, then "Smoothing" designs can be used to efficiently produce a meta-model of a simulation that is made up of a complex series of physical models